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Understanding Complexity in Natural, Built, and Social Systems: deriving fundamental insights on systems comprising multiple interacting elements

Identifying general principles and laws that characterize complexity and capture the essence of complex systems is one of the major challenges of 21st century science and engineering. Complex systems are more than just complicated; they display distinct characteristics not encountered in "simple" systems, such as multi-scale interactions, emergent behavior, pattern formation, and self-organization, and they are often inherently stochastic or operate in unpredictable settings. Nonlinear couplings and feedbacks across multiple processes and scales typify these systems. They are not amenable to reductionism; finding constructs that persist through the dynamics is fundamental, and involves a major role for innovative computational experimentation. As well as advancing science and engineering, the understanding of complexity will enable the design, synthesis, and control of novel complex engineered systems. Furthermore, it will facilitate intervention in and analysis of complex natural and social systems. This theme therefore promotes the exploration and modeling of natural interactions, connections, complex relations, and interdependencies, scaling from sub-particles to galaxies, from subcellular to biosphere, and from the individual to the societal, across time, in order to understand, mimic, synthesize, and exploit complex systems.

The functionalities offered by computational thinking allow "experiments" to take place entirely in cyberspace. In many situations, simulation through computation is the only feasible approach to a systematic investigation of realistic complex scientific phenomena, or is essential to the scientific basis for and design of "traditional" experiments. Key challenges include accuracy and resolution, efficiency, perturbation analysis, uncertainty, stochasticity, validation against "ground truth", long-term dynamics, and predictive modeling. Simulations and computational experiments in mainstream and informal education can engage students and the public in the excitement of scientific and engineering discovery.

Much of the understanding of complexity will come from mathematical and statistical modeling and analysis, based on both theoretical and empirical studies. Mimicking and synthesizing systems will exploit a wide variety of techniques. Complexity often requires advances in numerical methods for differential, algebraic, and discrete systems. Other approaches include agent-based modeling, neural networks, and dynamically interactive human-in-the-loop calculations. An important consideration for large systems is that scalable methods and tools be available in the working environments of scientists, engineers, and STEM educational researchers.